Microcanonical Simulation of Complex Actions: The Wess Zumino Witten Case

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Abstract

We present the main results of our microcanonical simulation of the Wess Zumino Witten action functional. This action, being highly non-trivial and capable of exhibiting many different phase transitions, is chosen to be representative of general complex actions. We verify the applicability of microcanonical simulation by successfully obtaining two of the many critical points of the Wess Zumino Witten action. The microcanonical algorithm has the additional advantage of exhibiting critical behaviour for a small 8×8 lattice. We also briefly discuss the subtleties that, in general, arise in simulating a complex action. Our algorithm for complex actions can be extended to the study of D-branes in the Wess Zumino Witten action.

1 Description and Results

In Minkowski spacetime, the Feynman path integral has a complex integrand given by e^{iS_M}, where S_M is the Minkowski action. On Euclidean continuation

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of spacetime, the integrand becomes real, namely, e^{-S_E}. The positive definite Euclidean action S_E is ideally suited for Monte Carlo simulations based on the canonical ensemble. There is, however, a class of actions that are generically of the form $S = S_R + iS_I$ in *both* Minkowski and Euclidean spacetime. These actions are of fundamental importance in physics, and we refer to them as complex actions. For example, all topological effects appear in the action in the form of complex actions. A chemical potential term renders the action complex. Lattice QCD at finite temperatures and and densities has a complex action, and so do chiral gauge theories. Complex actions appear in study of non-Hermitian hamiltonians, complex Langevin processes, random matrix models and so on.

A complex valued action does not have any probabilistic interpretation, and hence, for example the Metropolis algorithm is unsuitable. All attempts to numerically simulate complex actions for quantum field theories have met with formidable difficulties [1, 2, 3] due to diverging errors arising from increasingly large volumes needed for obtaining the continuum limit. In particular, the conventional Metropolis algorithm fails for complex actions due to large errors in simulating the expectation values of cosines and sines of extensive quantities. These expectation values are necessary due to the presence of the imaginary component in the action.

There have been some studies that simulate complex actions using the Langevin equation; however, the results of these simulations cannot be shown to converge to the required distribution [4, 5]. Other methods [6] also suffer from either a restriction to a very small lattice, or are not efficient or well defined.

In our work, we work directly with the Feynman path integral formulation of quantum field theory. We apply a generalized form of the microcanonical method to the case of complex actions. The microcanonical method has been very successful in simulating global quantities of real statistical systems [7, 8, 9]. The microcanonical method yields a direct computation of the partition function (up to a proportionality constant) and hence the determination of its (complex) zeros. The zeros themselves contain useful information, in particular whether the system has critical points. The microcaconical simulation technique therefore offers an attractive alternative to the usual methods, based on the canonical ensemble, for determining the phase diagram of statistical systems.

In this paper we extend the microcanonical algorithm to complex actions, and, compute its partition function. In particular, we study the well known

and highly nontrivial Wess Zumino Witten (WZW) complex valued action functional. Since this model exhibits many distinct phase transitions, we are able to provide a solid test of our algorithm. Our simulations **predicts** the critical parameters, and we confirm the effectiveness and accuracy of our simulation by comparing the simulated results with the known analytical results.

The Wess Zumino Witten action in two-dimensional Euclidean space has the following form

$$S = S_\lambda + ikS_I, \tag{1}$$

where the chiral term is given by

$$S_\lambda = \frac{1}{4\lambda^2}\int d^2x Tr(\partial_\mu g \partial_\mu g^{-1}) \tag{2}$$

and the imaginary piece comes from the Wess Zumino term

$$S_I = \frac{1}{24\pi}\int\limits_{S_3} d^3y \epsilon_{ijk} Tr[\bar{g}^{-1}\frac{\partial \bar{g}}{\partial y^i}\bar{g}^{-1}\frac{\partial \bar{g}}{\partial y^j}\bar{g}^{-1}\frac{\partial \bar{g}}{\partial y^k}]. \tag{3}$$

For the quantum field theory to be well defined, k must be integer-valued.

For the case of $SU(2)$, the Wess Zumino term can be parametrized in terms of the Euler angles [10], namely,

$$S_I = \frac{1}{\pi}\int d^2x \phi(x) sin^2\psi(x) sin\theta(x) \epsilon^{\mu\nu}\partial_\mu\psi(x)\partial_\nu\theta(x). \tag{4}$$

As is well known, the WZW model has infinitely many critical points, one for each integer value for k. The WZW model is conformally invariant at the critial coupling constants given by[10]

$$\lambda_c^2 = \frac{4\pi}{k} \quad ; \quad \text{k : integer.} \tag{5}$$

By extending the Lee-Yang theorem for zero's of the partition function to the complex case, we expect that the partition function, in the infinite volume limit, will be zero close to the critical coupling constants. We should be able to locate a zero (close to the continuum model) if the size of the lattice is large enough.

By calculating the simulated partition function as a function of k, the zeroes can be identified as the points of the k axis where the partition function

Z crosses over from a positive to a negative value. This cross over is a unique feature of complex actions, since the partition function of a real action can never be negative. Given that only integer k's are physical, the only physical zeros of Z are those that are close to integer values of k.

The partition function of the Wess Zumino Witten action functional is given by

$$Z(\lambda, k) = \int [DU] \exp(-S_\lambda) \exp(ikS_I), \tag{6}$$

which in turn can be cast into the form

$$Z(\lambda, k) = \int_{-\infty}^{+\infty} dE \rho(\lambda, E) \exp(ikE) \tag{7}$$

with the density of states given by

$$\rho(\lambda, E) = \int [DU] \delta(E - S_I) \exp(-S_\lambda) \tag{8}$$

The density of states is estimated by a generalization of the microcanonical algorithm. First, the simulation space is broken up into energy bins of size $\triangle E$. Bin $E = 0$ is taken to be the reference bin. The system is thermalized by randomly generating configurations and accepting only those configurations whose values of S_I fall within the first two bins. The density of states $\rho(\lambda, \triangle E)$ is estimated by calculating the occupation number ratio between the two bins. The updating of configurations and crediting of counts to the bins are based on a *combination* of the microcanonical and canonical ensembles. This is done as follows.

1. A new configuration is generated, and its acceptance is weighted by the usual Metropolis factor $\exp(-S_\lambda)$. Note that since the chiral contribution, being real, plays the role of a weighting action, the value of λ has to be at the **critical value** for a particular level; otherwise, if $\lambda \neq \lambda_c$, the system would never go critical.

2. The updated configuration is accepted only if it's S_I value falls within the two bins. If this is so, the counter for the bin where S_I lands is credited.

3. If the updated configuration does not satisfy the above criterion, a count will still be credited to the bin of the **old** configuration.

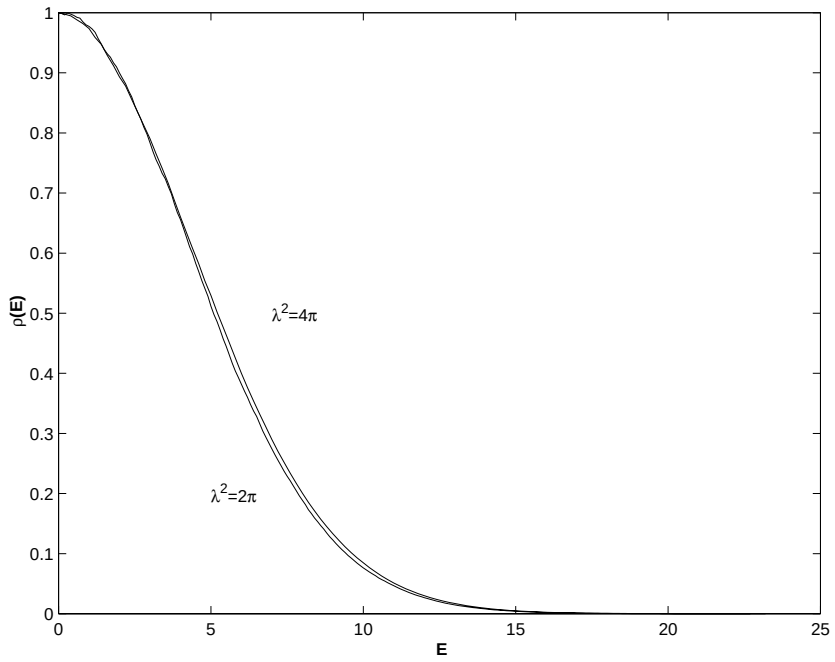

Figure 1: Density of states for two values λ_c

By continuing this process across all the energy bins allows us to get an estimation of the density of states. A crucial point in going from one set of bins to another is to have, in between, at least one overlapping bin for the purpose of normalizing the occupation number of the various bins.

All of the results quoted are for simulations for a 8×8 lattice, as this size is sufficient for accurately estimating the value of critical k. In our work, we tested our simulations for two levels, namely $k = 1$ and $k = 2$. For the critical coupling $\lambda_c^2 = 4\pi, \triangle E$ was set to be 0.2 while a finer value of 0.1 was chosen for $\lambda_c^2 = 2\pi$. A total number of about 1 million configurations were generated for every set of energy bins. The energy bin was terminated when the resulting density of state is less than 3 decimal places (which is the achieved level of accuracy in our simulations). The results for the simulated density of states is shown in Figure 1.

Since $\rho(\lambda, -E) = \rho(\lambda, E)$, it is only necessary to perform the simulation for $E \geq 0$. This reflection symmetry ensures that the WZW partition

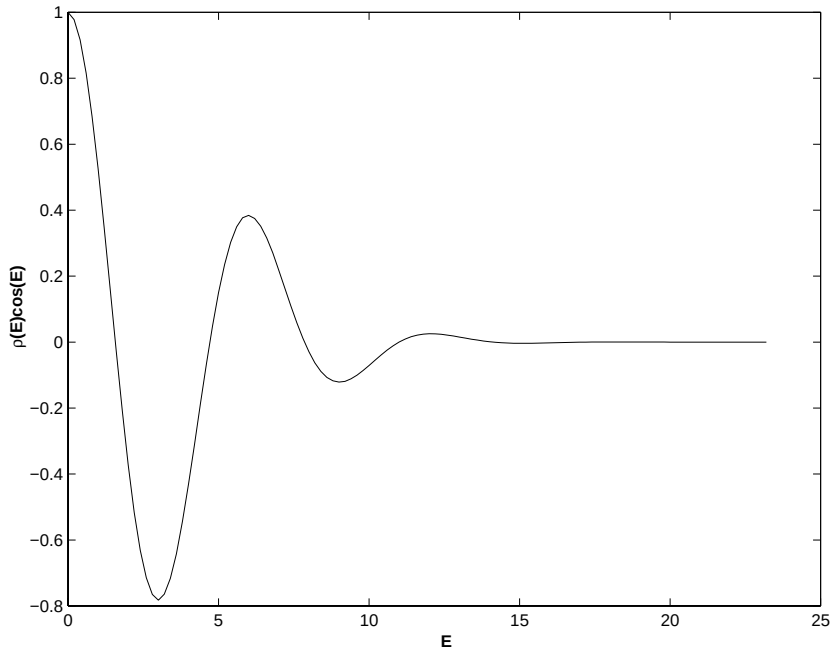

Figure 2: The integrand of Z for $\lambda_c = 4\pi$

function is real, since it simplifies to

$$Z(\lambda, k) = 2\int_0^\infty dE\rho(\lambda, E)cos(kE) \tag{9}$$

The simulated value for integrand of $Z(\lambda_c, k)$ is given in Figures 2 and 3. The plot of $Z(\lambda_c, k)$ against k is physical relevant only for integer k's. We expect that $Z = 0$ at the value of k that corresponds to $\lambda_c^2 = \frac{4\pi}{k}$; for other values of integer k, Z is physical and contains information on how the theory behaves away from criticality.

The behaviour of Z near its zero is given in Figures 4 and 5. By scanning for zeros of the simulated partition function Z that are close to integers, we find that:

$$k_{\text{simulated}} = 1.06 \pm 0.07 \quad (\text{for } \lambda^2 = 4\pi)$$

and

$$k_{\text{simulated}} = 1.95 \pm 0.06 \quad (\text{for } \lambda^2 = 2\pi).$$

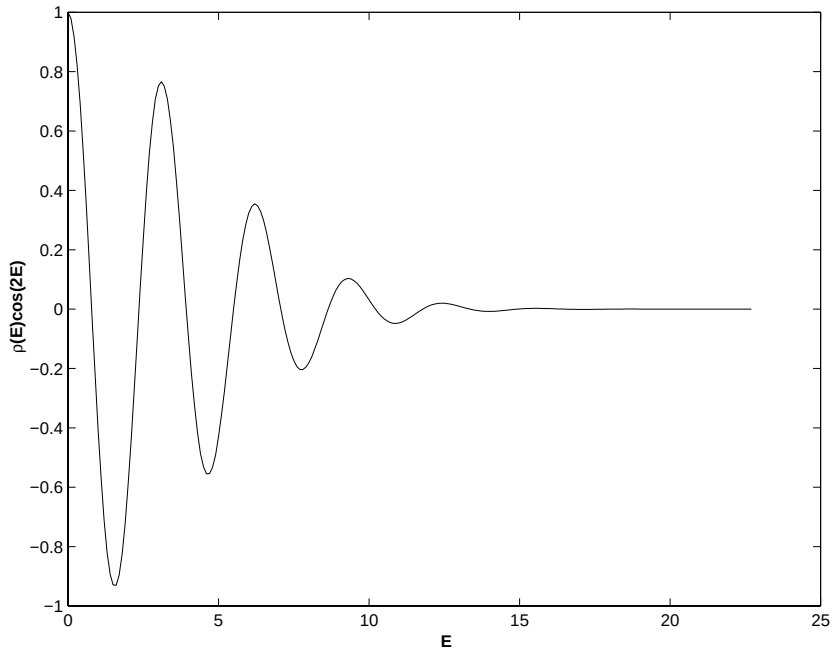

Figure 3: The integrand of Z for $\lambda_c = 2\pi$

The errors were deduced from the standard deviation computed from two separate sets of results for each coupling.

The exact values are $k = 1$ and $k = 2$ respectively, and we see that we have obtained a result of fairly high accuracy with a surprisingly small lattice.

2 Discussion

Our simulations of the Wess Zumino Witten action demonstrates that the microcanonical method is in principle capable of simulating complex actions. Unlike the case of real actions, however, there are several subtleties involved. Chief among them are the following.

1. A high degree of accuracy is required in order to achieve stable and consistent results. The reason being that, unlike real actions, terms in the complex action partition function **cancel** each other (see the

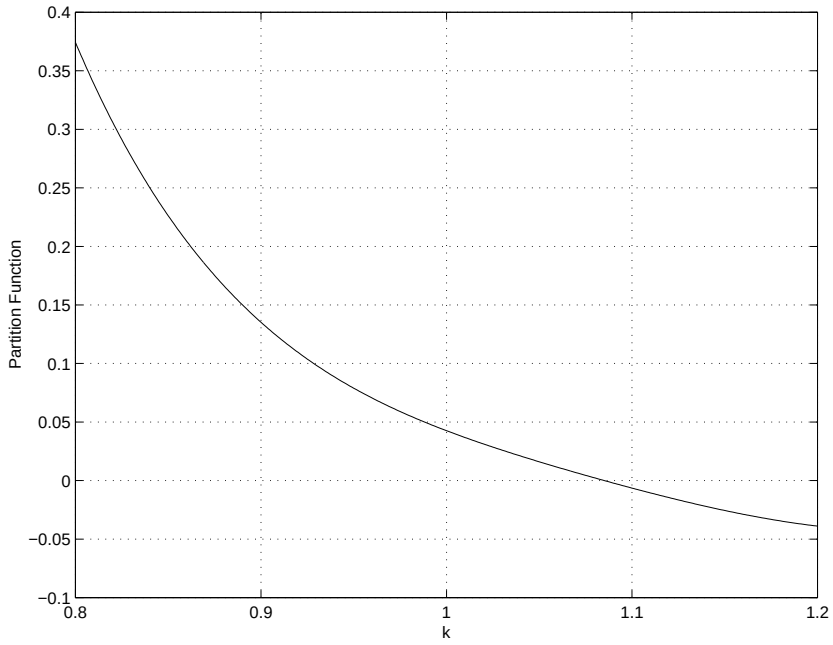

Figure 4: Scan of Z near a zero for $\lambda_c = 4\pi$. The zero occurs at $k \simeq 1.08$.

graphs of Figures 2 and 3), leaving behind a small value in the region where the phase transitions take place.

2. The fact that the critical point can be made to move from $k = 1$ to $k = 2$ by changing the value of λ_c in the weighting function is strong evidence that our simulation is giving the correct result. There are infinitely many critical points of the WZW model, one for each integer k, and in principal, all these critical points can be obtained by our simulation.

3. There is an additional necessity of having to provide a good resolution of the $\cos(kE)$ term. Typically, this means that there should be at least a few points within each trigonometrical quadrant. Consequently, since $\triangle E \sim \frac{1}{k}$, a smaller energy spacing is required for larger couplings. Computational time therefore is expected to increase as coupling k increases.

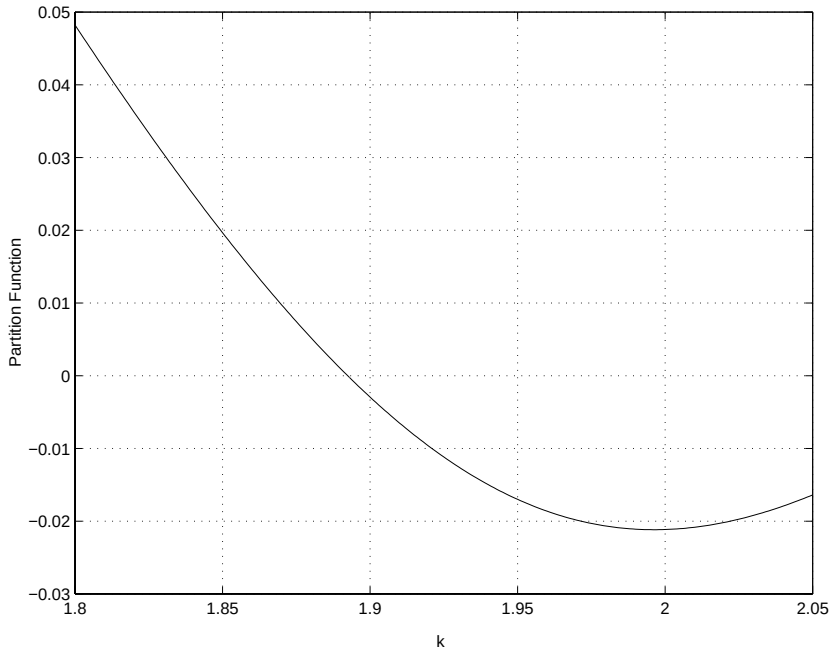

Figure 5: Scan of Z near a zero for $\lambda_c = 2\pi$. The zero occurs at $k \simeq 1.89$.

4. Since the cosine of an argument cannot be taken as a reliable weight in any Monte Carlo simulation, the contribution to the weight must always come from the real action. This constraint demands that the coupling λ in the real action has to be fixed at its critical value λ_c. In other words, it is not possible to fix the coupling in the imaginary component, namely k, and deduce the critical coupling λ_c of the real action.

5. Our method is ideally suited for studying the critical properties of extended systems. In particular, D-branes in the WZW model are non-local background configurations that respect the conformal invariance of the theory [11]. Our method, for example, can numerically study under what circumstances a D-brane background in the WZW model results in a conformally invariant system.

In conclusion, we believe that the ability of the microcanonical technique to get accurate predictions from the Wess Zumino Witten action is a major

step forward in the simulation of complex actions, and opens the way for numerically studying other complex actions, as well as extended objects such as D-branes.

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